

# Molecular production at a wide Feshbach resonance in Fermi-gas of cooled atoms.

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The problem of molecular production from degenerate gas of fermions at a wide Feshbach resonance, in a single-mode approximation, is reduced to the linear Landau-Zener problem for operators. The strong interaction leads to significant renormalization of the gap between adiabatic levels. In contrast to static problem the close vicinity of exact resonance does not play substantial role. Two main physical results of our theory is the high sensitivity of molecular production to the initial value of magnetic field and generation of a large BCS condensate distributed over a broad range of momenta in inverse process of the molecule dissociation.

In recent years there have been numerous achievements in the area of ultra-cold atomic physics. The major experimental tool for it is the use of the Feshbach resonances (FR) [1, 2, 3, 4, 5, 6, 7], which occurs when the energy of a quasibound molecular state becomes equal to the energy of two free alkali atoms. The magnetic-field dependence of the resonance allows precise tuning of the atom-atom interaction strength in an ultracold gas [1]. Moreover, time-dependent magnetic fields can be used to reversibly convert atom pairs into weakly bound molecules [8, 9, 10, 11, 12, 13, 14, 15]. This technique has proved to be extremely effective in converting degenerate atomic gases of fermions [8, 9, 10, 11, 16, 17, 18] and bosons [14, 15, 19] into bosonic dimer molecules.

The Feshbach resonance proceeds at sufficiently strong magnetic fields so that electronic spins are polarized. The collisions in s-channel of such Fermi-atoms is possible only if they have different states of nuclear spins. In a typical experiment [8, 17] an admixture of atoms of  $^{40}\text{K}$  with the same total atomic spin  $9/2$  but different spin projection quantum numbers  $-7/2$  and  $-9/2$  was used.

Theoretical works on the molecular production can be roughly divided in two categories. The first is a phenomenology suggesting that the pairs of molecules perform independently the Landau-Zener (LZ) transitions [4, 6]. Therefore the total number of molecules in the end of the process is the LZ transition probability multiplied by the number of pairs. The most problematic in this approach is what should be accepted for the LZ transition matrix element  $\Delta$  (further we call it the LZ gap). Direct calculation of the transition probability from a microscopic Hamiltonian up to the 4-th order in the interaction constant [20] shows that, in contrast to the assumption of phenomenological works, the many-body effects are very essential. Another category includes the works based on a simplified model [21], in which molecules have only one available state mimicking the condensate [22, 23, 24]. Though the numerical works of this category displayed a reasonable temperature dependence, they could not give a clear physical picture and detailed dependencies on parameters of the problem. The series of semi-analytical works by Pazy *et al.* [22, 25, 26, 27] were based on two contradicting assumptions as we show later.

In this letter we consider the process of molecule production from fermi-gas of atoms after the FR is swept across the Fermi sea. The accepted model is valid under assumption of strong interaction equivalent to the condition of wide resonance [28]. We derive the closed equation for such process. We show that the problem of molecular production from degenerate gas of fermions in a single-mode approximation can be reduced to the linear LZ problem for operators. In this respect our result agrees with the conjecture of the phenomenological theories, but the strong interaction leads to significant renormalization of the LZ gap, which occurs to be independent on the fermi-gas density. Our results display a significant dependence of the molecular production on the initial state preparation. At the inverse transformation of the BEC molecular gas into atomic gas the latter appears in the state with strongly developed BCS condensate directly after magnetic field sweeping.

Our starting point is the Timmermanns *et al.* Hamiltonian [31]

$$\hat{H} = \sum_{p,\sigma} (\epsilon(t) + \epsilon_p) \hat{a}_{p\sigma}^\dagger \hat{a}_{p\sigma} + \sum_p \omega_p \hat{b}_p^\dagger \hat{b}_p + \frac{g}{\sqrt{V}} \sum_{p,q} \left( \hat{b}_q \hat{a}_{p+q\uparrow}^\dagger \hat{a}_{-p\downarrow}^\dagger + \hat{b}_q^\dagger \hat{a}_{-p\downarrow} \hat{a}_{p+q\uparrow} \right) \quad (1)$$

describing fermionic atoms, created by  $\hat{a}_{p\sigma}^\dagger$  with momentum  $p$ , spin  $\sigma = \uparrow, \downarrow$  which distinguishes between the two internal states of the atoms, and kinetic energy  $\epsilon_p$ , that are coupled to diatomic bosonic molecules with kinetic energy  $\omega_q$  created by  $\hat{b}_q^\dagger$ . The position and the width (molecular lifetime) of the FR are respectively controlled by the bare time-dependent detuning energy  $\epsilon(t)$  and the coupling constant  $g$ , the former experimentally tunable by magnetic field. The Hamiltonian (1) neglects nonresonant atom-atom and molecule-molecule interactions that near a FR are subdominant to the resonant scattering.

In this letter we use the word "atoms" for both, uncoupled atoms and those inside molecules, and the word "fermions" for atoms that are not bound in molecules. Correspondingly, we denote the number of atoms  $\hat{N}$  and the number of fermions  $\hat{N}_F$ .

First we demonstrate that the condition of wide res-

onance allows to neglect kinetic energy of fermions. Indeed, the calculations in weak coupling approximation [20] show that the characteristic interaction energy is  $g\sqrt{n}$ , where  $n = N/V$  is the density of atoms. If  $g\sqrt{n}$  exceeds the Fermi energy of fermions  $\epsilon_F = \hbar^2(3\pi^2n)^{2/3}/2m$  the fermion dispersion can be neglected. This requirement is equivalent to:

$$\Gamma = \frac{(2mg/\hbar^2)^2}{(3\pi^2)^{4/3}} n^{-1/3} \gg 1 \quad (2)$$

which coincides with the definition of the wide resonance [28]. The same criterion allows to neglect the dispersion of molecules. This approximation has been used earlier [26, 29] and numerical proof of its validity has been reported in [27].

In what follows we assume that only molecules with zero momentum  $\hat{b}_{q=0}^\dagger$  are produced, neglecting molecules  $\hat{b}_{q \neq 0}^\dagger$  excited above the molecular condensate (the single-mode approximation). This assumption was justified for the equilibrium state in the case of wide resonance [28] and used in the most of theoretical works on the dynamics of transition [5, 25, 26, 27, 29]. We thus replace  $\hat{b}_q$  in Eq. (1) by  $\hat{b}_0\delta_{q,0} \equiv \hat{b}\delta_{q,0}$ . With this simplification one notices that only a pair of fermions with opposite momenta and spin can be converted into a molecule. The two assumptions allow to simplify the Hamiltonian (1) and to solve the problem exactly.

Let us introduce spin operators  $\hat{S}_z, \hat{S}_-$  and  $\hat{S}_+ = \hat{S}_-^\dagger$  as follows:

$$\hat{S}_z = \frac{1}{2} \sum_p (\hat{n}_{p\uparrow} + \hat{n}_{-p\downarrow} - 1) \quad \hat{S}_- = \sum_p \hat{a}_{p\uparrow} \hat{a}_{-p\downarrow}; \quad (3)$$

with the standard commutation relations  $[\hat{S}_+, \hat{S}_-] = 2\hat{S}_z$ ,  $[\hat{S}_z, \hat{S}_+] = \hat{S}_+$ . Neglecting fermion and Boson kinetic energy one can rewrite the Hamiltonian (1) in terms of spin operators:

$$\hat{H} = 2\epsilon(t)\hat{S}_z + \frac{g}{\sqrt{V}} (\hat{b}\hat{S}_+ + \hat{b}^\dagger\hat{S}_-) \quad (4)$$

This Hamiltonian commutes with the operator  $\hat{Q} = \hat{S}_z + \hat{b}^\dagger\hat{b}$  equivalent to the total number of atoms  $N$  and additionally with the square of total spin operator  $\mathbf{S}^2 = S_z^2 + S_+S_- - S_z$ . It follows from the first equation (3) that  $S_z = (\hat{N}_F - N_s)/2$ , where  $\hat{N}_F$  is the number of fermions and  $N_s$  is the number of available fermionic states. Thus,  $\hat{Q} = (\hat{N} - N_s)/2$ . Since  $N_s \gg N \geq N_F$  we can approximate  $S_z \approx -N_s/2$ .

The Heisenberg equations of motion are:

$$\hbar\dot{\hat{b}} = -i\tilde{g}\hat{S}_-; \quad \hbar\dot{\hat{S}}_- = -2i\epsilon(t)\hat{S}_- + 2i\tilde{g}\hat{b}^\dagger\hat{S}_z \quad (5)$$

Generally these equations are non-linear. However, in the wide-resonance approximation  $S_z = -N_s/2$ , they become linear. Eliminating  $\hat{S}_-$ , we arrive at an ordinary linear differential equation for the operator  $\hat{b}$ :

$$\hbar^2\ddot{\hat{b}} + 2i\hbar\epsilon(t)\dot{\hat{b}} + \Delta^2\hat{b} = 0 \quad (6)$$

where  $\Delta = g\sqrt{n_s}$  and  $n_s = N_s/V$  is the density of available states. Linear equation (6) turns into the parabolic cylinder equation if  $\epsilon(t)$  is a linear function of time. In the LZ theory it describes the evolution of the amplitude to find the system in one of its two states. The role of the LZ gap is played by the value  $\Delta = g\sqrt{n_s}$ , which strongly exceeds  $g\sqrt{n}$ . The characteristic time during which the LZ transition takes place  $\tau_{LZ}$  is determined by requirement that the instantaneous frequency  $2\epsilon(\tau_{LZ})$  becomes equal to  $\Delta$ . Thus, the characteristic value of  $\epsilon(t)$  is equal to  $\Delta = g\sqrt{n_s} \gg \epsilon_F$ .

The model neglecting the dispersion is valid until the kinetic energy  $\frac{p_s^2}{2m} \ll g\sqrt{n_s}$ . The value  $p_s$  limiting available states is determined by equation:

$$\frac{p_s^2}{2m} = g\sqrt{n_s} \quad (7)$$

and the density of available states  $n_s$  is associated with the limiting momentum  $p_s$  by a standard relation:

$$n_s = \frac{(p_s/\hbar)^3}{3\pi^2} = \frac{(2mg/\hbar^2)^6}{(3\pi^2)^4} = n\Gamma^3; \quad (8)$$

Both  $n_s$  and  $\Delta$  are independent on the density of fermions  $n$ . The condition of the wide resonance (2) requires that  $N_s \gg N$  thus justifying the accepted approximation. In a series of works by Pazy, Tikhonenkov *et al.* [26, 27], the authors neglected dispersion and put  $N_s = N$ . As it was demonstrated above the neglecting of dispersion is justified only if the condition of the wide resonance (2) is satisfied. But the same condition ensures that  $N_s \gg N$ . Thus, their two fundamental assumptions physically contradict each other, though their model is mathematically consistent. Exact quantum solution of the same problem was recently found by Altland and Gurarie [32].

The value  $g$  can be extracted from the experimental data on the dependence of the scattering length on magnetic field near the FR [30] using a well-known relation:  $g = \hbar\sqrt{4\Pi(a-a_0)\epsilon}/m$ . On the other hand it can be estimated theoretically as  $g \sim \epsilon_{hf}\sqrt{a_0^3}$ , where  $\epsilon_{hf}$  is the hyperfine energy and  $a_0$  is the radius of the molecule far from the resonance. Both these estimates give for  $^{40}\text{K}$   $g \sim 10^{-28} \text{ erg} \times \text{cm}^{3/2}$  and  $\Delta = 0.006 \text{ K}$ . The sweeping of magnetic field proceeds with amplitude few hundred Gauss. It corresponds to energy scale about  $0.03 \text{ K}$ , larger than  $\Delta$ .

The first important conclusion is that the dynamic LZ problem is simpler than the static equilibrium one. In the latter problem most interesting and intriguing phenomena take place at very small  $\epsilon \leq \epsilon_F$ . In this range of energy the s-scattering amplitude reaches its unitary limit and scattering length changes sign resulting in strong

BCS coupling and complex behavior of the atomic and molecular densities. It is not the case in the dynamic problem since the effective interval for transformations of atoms into molecules is  $\Delta \gg \varepsilon_F$ . This statement is correct for any sweeping rate above relaxation.

Another important conclusion is that the strong interaction leads to renormalization of the LZ gap. The energy scale which appears in the perturbation theory is  $\Delta^{(0)} = g\sqrt{n}$  [20]. In the case of wide resonance  $\Delta = g\sqrt{n_s}$  is much larger than  $\Delta^{(0)}$  and does not depend on the density of atoms.

Employing equations (5), the general solution of the ordinary differential equation (6) reads:

$$\hat{b}(t) = u(t, t_0) \hat{b}(t_0) - i\tilde{g}v(t, t_0) \hat{S}_-(t_0), \quad (9)$$

$$i\tilde{g}\hat{S}_-(t) = -\dot{u}(t, t_0) \hat{b}(t_0) + i\tilde{g}\dot{v}(t, t_0) \hat{S}_-(t_0), \quad (10)$$

where  $u(t, t_0)$  and  $v(t, t_0)$  are standard solutions of the same equation satisfying initial conditions  $u(t_0, t_0) = 1$ ,  $\dot{u}(t_0, t_0) = 0$  and  $v(t_0, t_0) = 0$ ,  $\dot{v}(t_0, t_0) = 1$ . These solutions have the following properties:

$$|u|^2 + \Delta^{-2} |\dot{u}|^2 = \Delta^2 |v|^2 + |\dot{v}|^2 = 1; \dot{u}^* \dot{v} + \Delta^2 u^* v = 0 \quad (11)$$

The solution (9,10) allows to follow the evolution of the number of molecules  $N_m(t) = \langle \hat{b}^\dagger \hat{b} \rangle(t)$ , the BCS condensate amplitude  $F(t)$  defined by equation  $F^2(t) = \langle \hat{S}_+ \hat{S}_- \rangle(t)$ , and the BCS-BEC coherence factor  $C(t) = \langle \hat{b}^\dagger \hat{S}_- \rangle(t)$ . In the case when initial coherence factor is zero it is given by:

$$N_m(t) = |u|^2 N_m(t_0) + \tilde{g}^2 |v|^2 F^2(t_0) \quad (12)$$

$$\tilde{g}^2 F^2(t) = |\dot{u}|^2 N_m(t_0) + \tilde{g}^2 |\dot{v}|^2 F^2(t_0) \quad (13)$$

$$C(t) = i\tilde{g}^{-1} \dot{u} u^* N_m(t_0) + i\dot{v} v^* F^2(t_0), \quad (14)$$

where  $\tilde{g} = g/\sqrt{V}$ . Using (11) and summing eqs. (12) and (13) we find that

$$N_s N_m(t) + F^2(t) = \text{const}, \quad (15)$$

which is a consequence of the conservation laws. Since for any state  $F^2(t) > 0$ , if there are no molecules in the initial state, their number  $N_m(t)$  can not exceed a value  $F^2(t_0)/N_s$  at any time. Therefore, the final molecule production rate depends on the initial state. Below we consider two experimentally most relevant situations: no molecules and only molecules and no fermions in the initial state. In both these cases the initial value  $C = \langle \hat{b}^\dagger \hat{S}_- \rangle(t_0) = 0$ .

In the case of no molecules in the initial state  $N_m(t_0) = 0$  general equations (12,14) simplify to

$$N_m(t) = \tilde{g}^2 |v|^2 F^2(t_0); \quad i\tilde{g}C(t) = -\tilde{g}^2 \dot{v} v^* F^2(t_0) \quad (16)$$

Evolution of  $F(t)$  in this case is completely determined by (15). Note, that the coherence factor  $C(t)$  does not remain zero. If at the initial moment there exists both

condensate of molecules  $\langle \hat{b} \rangle$  and the BCS condensate  $\langle \hat{S}_- \rangle$ , their time evolution can be obtained from equations (9,10) by taking averages from both sides.

The value  $F^2(t_0)$  strongly depends on the initial state. We consider first an initial state defined as the filled Fermi sphere. The condensate density can be readily found for this state:  $F^2 = N/2$ . Thus, the final average number of molecules in this case is very small  $N_m(+\infty) \leq N/(2N_s)$ . To produce a reasonable fraction of molecules it is necessary to have large condensate amplitude in the initial state. A natural way to generate such initial state is to start with sufficiently small negative detuning energy  $\epsilon$ . The effective dimensionless BCS coupling constant reads  $\lambda_{BCS} = -\nu_F g^2/\epsilon$ , where  $\nu_F$  is the density of state at the Fermi-energy [28]. This constant becomes of the order of 1 at  $|\epsilon| \sim \Gamma\epsilon_F$ , a value of detuning between Fermi-energy and the gap  $\Delta$ . When detuning becomes less than this value the condensate spreads from an exponentially narrow spherical layer near the Fermi sphere to a sphere of the radius given by the cut-off momentum  $p_c$ . The latter is inverse proportional to the effective radius of the hyperfine interaction and is much larger than  $p_s$ . Therefore, the molecular production determined by the part of initial BCS condensate confined in the sphere of the radius  $p_s$  first grows and then decreases when the initial detuning decreases.

Such a strong dependence of the final molecular production on the initial state, in particular on the value of the initial magnetic field explains why different experimenters obtain different fractions of molecules in the final state even in the adiabatic regime [9, 12, 17, 18]. Note, that in experiments in which a significant molecular production was achieved the initial state was indeed close to the FR, whereas the final state could be sufficiently far from it.

Thus, in a realistic experimental setup the initial value of  $\epsilon$  is small  $\epsilon_0 \leq \Gamma\epsilon_F \ll \Delta$  and then  $\epsilon$  increases linearly with time. In this case one can put  $t_0 = 0$ , and  $\epsilon(t) = \dot{\epsilon}t$ . Equation (6) turns into the parabolic cylinder equation. Its standard solution  $u(t, 0)$  has an asymptotic property:  $|u(\infty, 0)|^2 = \exp(-\pi\Delta^2/2\hbar\dot{\epsilon})$ . Employing it together with (11) and (16), we arrive at the following number of molecules in the final state:

$$N_m(+\infty) = F_0^2 N_s^{-1} [1 - \exp(-\pi\Delta^2/2\hbar\dot{\epsilon})] \quad (17)$$

It can be proven that the maximal possible value of  $F^2$  is  $N_s N/2$ . It corresponds to complete transformation of atoms into molecules in the adiabatic regime  $\dot{\epsilon} \rightarrow 0$ . Equation (17) looks exactly as the LZ transition probability multiplied by an effective number of pairs, but in contrast to phenomenological theories [4, 6] and the perturbation theory result [20] the coefficient in front of  $1/\dot{\epsilon}$  in exponent does not depend on the initial density of the atoms. This theoretical prediction can be checked experimentally.

Finally, we consider an inverse process with no fermions, no BCS condensate and only the molecular condensate in the initial state:  $\langle \hat{b} \rangle(-\infty) = \sqrt{N/2}$  and sweeping of the magnetic field in opposite direction. Then in the end the condensate density is determined by the LZ value:  $\langle \hat{b} \rangle(+\infty) = \sqrt{N/2} \exp(-\pi\Delta^2/2\hbar\dot{\epsilon})$ , whereas the absolute value of the BCS condensate amplitude  $\langle \hat{S}_- \rangle$  can be found from the conservation law (15):

$$|\langle \hat{S}_- \rangle|^2 = \frac{N_s N}{2} \left[ 1 - \exp\left(-\frac{\pi\Delta^2}{\hbar\dot{\epsilon}}\right) \right] \quad (18)$$

This result has a clear physical interpretation. It corresponds to  $\frac{N}{2} [1 - \exp(-\pi\Delta^2/\hbar\dot{\epsilon})]$  Cooper pairs distributed with identical probability  $w = \frac{N}{2N_s} [1 - \exp(-\pi\Delta^2/\hbar\dot{\epsilon})]$  between  $N_s$  available states. Then the modulus of the pair amplitude at a fixed state is  $\langle \hat{a}_{\mathbf{p}\uparrow} \hat{a}_{-\mathbf{p}\downarrow} \rangle = \sqrt{w}$ . If all these amplitudes have the same phase, the total condensate amplitude is equal to  $\langle \hat{S}_- \rangle = N_s \sqrt{w}$ , which is equivalent to equation (18). This result has experimentally verifiable consequence. Indeed, the pair created after the sweeping of magnetic field has the size in real space  $r_{pair} = \frac{\hbar}{p_s} \ll n^{-1/3}$ . It means that the pair is a compact formation well separated from other pairs and, therefore, can be rather qualified as a quasimolecule. In contrast to real molecules the quasimolecules have parallel electron spins. The second their peculiarity is their instability: after the sweeping of magnetic field stops, they decay during the relaxation time. The latter is rather long since the pair fermion collisions do not produce energy relaxation. The experimental estimate for the relaxation time is in the range of seconds. Therefore, it seems quite feasible to switch off the trap for much shorter time and observe the correlations of momenta and spins in runaway particles. The prediction of our theory is that the correlation prefers opposite velocities and parallel spins in the range of energy up to  $\Delta$ .

In conclusion, we considered the molecule formation and dissociation in cooled Fermi-gas when magnetic field is swept across the wide Feshbach resonance. It was demonstrated that in this situation the fermion kinetic energy is negligible. The resulting molecular production from initial fermions is described by LZ-like formulae with strongly renormalized LZ gap independent on the density of initial fermions. However, the molecular production strongly depends on initial value of magnetic field. In the inverse process of molecular dissociation immediately after the sweeping stops, there appear Cooper pairs with parallel electronic spins and opposite momenta homogeneously distributed within a sphere in the momentum space, whose radius  $p_s$  is much larger than the Fermi momentum. Another experimentally verifiable prediction is independence of the coefficient in front of  $1/\dot{\epsilon}$  in LZ exponents entering the equations for molec-

ular production (17) and the BCS condensate amplitude (18) on the initial density of atoms (molecules).

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